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ScienceDirect

Energy Procedia 76 (2015) 444 – 453

Energy Procedia

European Geosciences Union General Assembly 2015, EGU

Division Energy, Resources & Environment, ERE

# Chemical process modelling of underground coal gasification and evaluation of produced gas quality for end use

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**Abstract**

The chemical process at the heart of Underground Coal Gasification (UCG) is the engineered injection of a blend of gasification (normally $O_2$, air, $H_2O$) agents into the coal resource. Established surface gasifier chemical modelling principles are adapted for modelling UCG processes. Model configurations developed in Aspen Plus are used to simulate the Linked Vertical Wells and the Controlled Retractable Injection Point gasifier layouts. Sensitivity analyses were conducted to investigate the effect of operational parameters and performance indicators. Model outputs were validated using reported UCG trial results. The gasification designs developed could form the basis for developing an integrated UCG model.



Peer-review under responsibility of the GFZ German Research Centre for Geosciences

*Keywords:* Chemical process modelling; Aspen Plus simulation; Underground Coal Gasification (UCG); Syngas; Coal

## 1. Introduction

Coal is one of the most commonly used fossil fuels which currently meets approximately 40% of the global electricity demand, while also covering one quarter of the global energy needs. However, these figures barely reflect the importance of coal as an energy source, considering that only 15 to 20% of the known coal resources are suitable for conventional raw material extraction through surface and underground mining [1]. Underground coal gasification (UCG), a method of gasifying coal in-situ and converting it to syngas, may offer a cost-competitive and sustainable

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Peer-review under responsibility of the GFZ German Research Centre for Geosciences
doi:10.1016/j.egypro.2015.07.870

alternative to conventional mining [2-4]. This is possible because UCG does not include any underground labour and reduces the machinery and equipment costs required, as compared to the conventional mining and surface coal gasification [5, 6], and, in addition, provides benefit from coal seams that would otherwise remain unexploited and inaccessible due to economic and safety concerns [6-8].

Notwithstanding the distinctive features of different UCG designs, the common feature of all configurations is purposefully engineered boreholes directed within the coal resource, which are used to supply a mixture of gasification reagents (normally $O_2$, air, $H_2O$) and collect the product gas. Following ignition, the reagents support the gradual transformation of the coal seam into syngas which is collected, transported to the surface and, depending on its composition (mainly $H_2$, CO, $CO_2$ and $CH_4$), can be used either as chemical feedstock or as fuel for power generation [5, 9-12]. The employment of directional drilling techniques to engineer the injection and production boreholes represents a significant advance, which is adopted from the oil and gas industry [9, 11].

The thermo-chemical processes that take place during the UCG syngas generation affect the composition of the product gas [11]. Research findings have highlighted the operational similarity between UCG and above ground fixed bed reactors [5, 13]. These processes involve homogeneous and heterogeneous reactions, as well as heat and mass transfer phenomena which take place during the development of the UCG cavity (the void created inside the seam as coal is consumed). Modelling the UCG operation is, therefore, a complex task which requires the integration of a number of diverse processes, including chemical processes related to coal gasification as well as thermal and transport processes for the syngas and fluids involved [8, 14-17].

In this paper, the focus is on modelling the chemical processes taking place during UCG progression, as a stepping stone in preparing a fully integrated UCG process modelling system. Different UCG layouts in essence involve different chemical process designs. These chemical processes form a crucial component of UCG modelling although they have attracted limited attention in earlier studies due to the uncertainties and the extensive computational requirements associated with such modelling. The influence of the UCG operating conditions upon these processes and the control that they exert on the product gas composition necessitate detailed work in order to ultimately integrate them in a multi-component UCG design. The work reported here presents the latest results from such efforts.

**Nomenclature**

| | |
|---|---|
| UCG | Underground Coal Gasification |
| LVW | Linked Vertical Wells |
| CRIP | Continuous Retracting Injection Point |

## 2. Methodology

The two UCG subsurface layouts discussed in this paper are the Linked Vertical Wells (LVW) and the Continuous Retracting Injection Point (CRIP) geometries. Both geometries belong to the shaft-less UCG methods [11, 18] although their operational details are distinctly different. The detailed consideration of the UCG subsurface gasifier layout is crucial for the development of a reliable process model that can be used to simulate the relevant chemical processes.

The geometry of the LVW design is presented in Fig.1. A linkage path can be formed inside the coal seam through reverse combustion, hydraulic fracturing or directional drilling, enhancing the flow of gas between the two vertical wells (production and injection). The injection of the gasification reagents as well as the initiation stage takes place close to the injection well, where the combustion face is located too. This face is moving gradually towards the production well leaving a growing cavity behind as the coal is consumed. The syngas product flows towards the production well, from where it is transported to the surface [18, 19]. This flow of product gas along the coal seam facilitates the heat exchange between the high temperature gas and the pyrolised coal before it becomes combusted [5]. The heat exchange is a crucial element of the chemical process model developed and it is a distinctive characteristic, as compared to other UCG geometries (e.g. CRIP). The CRIP geometry is presented in

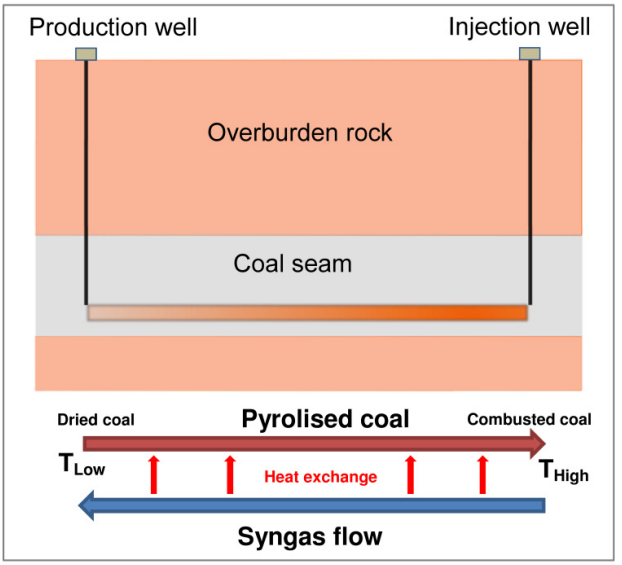


Fig. 1. Linked Vertical Well subsurface gasifier vertical cross-section.

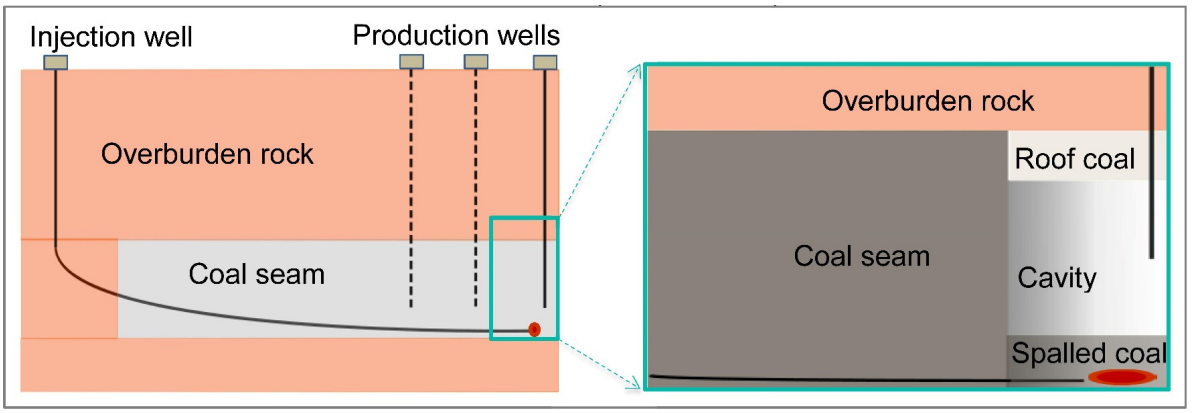


Fig. 2. Continuous Retracting Injection Point (CRIP) subsurface gasifier vertical cross-section.

Fig. 2. In the CRIP layout the injection well is directionally drilled horizontally along the bottom of the coal seam reaching close to the initial production well [20].

This injection well sustains the gasification process by supplying the gasifying agents. As the gasification proceeds and a localised cavity is created, the injection well can be retracted backwards facilitating the reaction of the gasifying agents fed with fresh coal [21, 22].

In addition, new vertical production wells are drilled closer to the fresh end of the horizontal injection well in order to transport the product gas generated to the surface, minimising its loss in the growing cavity as coal is consumed [22]. The CRIP geometry, compared to the LVW design, offers higher coal seam exploitation efficiency since it increases the controllability of the gasification process with the retracting injection well [23].

Although existing literature [5, 13] has highlighted the similarities of UCG operation with fixed bed gasifiers, limited attention has been paid on how specific subsurface layouts can be associated with surface gasification

processes. For instance, different thermodynamic conditions (e.g. temperature) are developed and different proportions of the injected oxidant reagents manage to successfully react with the coal under different UCG designs. Unavoidably, such differences lead to different product gas compositions. In this paper, the Aspen Plus® software simulation tool is employed in order to facilitate the simulation of the chemical processes and the process model configuration is tailored to specific UCG layouts.

## 3. Model Development

The chemical process simulation models developed in this work group the UCG reactions in four zones. These are the drying, pyrolysis, gasification and combustion zones in line with classifications used to study the chemistry of UCG [5, 16, 24]. Similar to previous process modelling efforts [25-28], the models detailed in this paper are composed of a number of streams and reactor compartments. The streams include both material and heat flows. The models consider that steady state conditions exist with perfect heat exchange between the reactor compartments followed by pressure balance during the process.

### *3.1. Linked Vertical Wells (LVW) – Process Model*

The LVW process model (Fig. 3) developed is characterised by the forward transfer of the coal mass through the stages of drying and pyrolysis before reaching the higher temperature gasification and combustion stages. Oxidant injection is performed in the combustion stage in order to induce the exothermic reactions of that step. Decomposition of coal to its components (according to its ultimate analysis) occurs at the pyrolysis stage and it is required since Aspen Plus® software recognises coal as a non-conventional element and, its handling requires coal to be broken down to its conventional compounds [25-31].

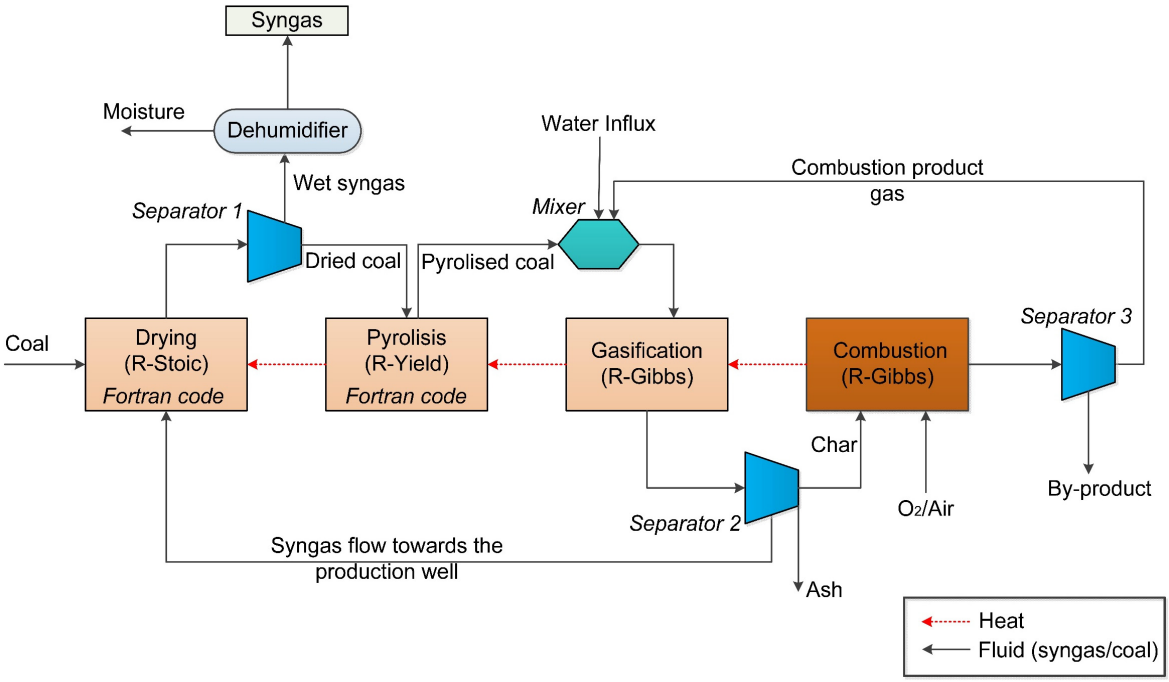


Fig. 3. Chemical process model for the simulation of the LVW subsurface layout.

In line with the LVW subsurface layout, the LVW process model developed (Fig. 3) illustrates that the collected syngas is produced at the higher temperature stages (i.e. combustion and gasification – that exist closer to the injection well) and passes through the coal seam reaching the lower temperature drying stage before it is collected and transported to the surface through the production well. During its flow, the high temperature syngas produced reacts with the cooler coal contributing to the necessary heat supply that is required for the endothermic reactions which take place at the drying and pyrolysis stages. In the model code prepared, both drying and pyrolysis stages are controlled through FORTRAN statements that define the operating parameters. The drying stage is simulated through a stoichiometric reactor (R-Stoic) while the pyrolysis (decomposition) stage through an R-Yield reactor. The gasification and combustion stages are formulated through R-Gibbs reactors. R-Gibbs reactors allow reactions to reach equilibrium based on minimisation of the Gibbs-free energy [25-28, 32].

### *3.2. Continuous Retracting Injection Point (CRIP) – Process Model*

Compared to the LVW subsurface layout, the CRIP geometry follows a different approach for the sequential gasification of coal blocks inside the coal seam. This process is implemented through the retracting injection point, which enables the gasification of a new part of the coal seam with every retraction [21, 22]. As a result, the CRIP process consists of multiple repetitive stages and its process model reflects how the syngas generation procedure works during a stage of this sequentially recurring process. More specifically, the CRIP process model (Fig. 4) allows the detailed investigation of how UCG gasification works at localised parts of the coal seam compared to the more macroscopic view given in the LVW model. The CRIP process model developed has been structured to reflect the vertical cross-section presented in Fig 2b; which is in line with literature depicting the CRIP UCG process [5, 8].

In the CRIP process model, the generated syngas is a mixture of the roof-stage and the bottom-gasification products (Fig. 4). Specifically, the roof coal is partially gasified during the roof-stage gasification (R-Gibbs reactor) after which part of the coal is converted to gas and part of it starts spalling in the developing cavity. The spalled coal is accumulated at the bottom together with rubble material, where the combustion and the bottom-stage gasification take place [5, 8]. In the cavity (reactor space), the roof-stage gas reacts with the bottom-stage gasification product before being collected through the production well. The combustion and gasification stages as well as the cavity reactions are simulated with R-Gibbs blocks following the R-Gibbs energy minimisation principle [25-28, 32]. Similar to the LVW process model, the injection of oxidants happens at the combustion stage. This injection facilitates the exothermic reactions taking place at the bottom of the cavity between the oxidants and the coal. In addition, the drying and pyrolysis stages within the process model are controlled with FORTRAN statements, similar to those used in the LVW process model.

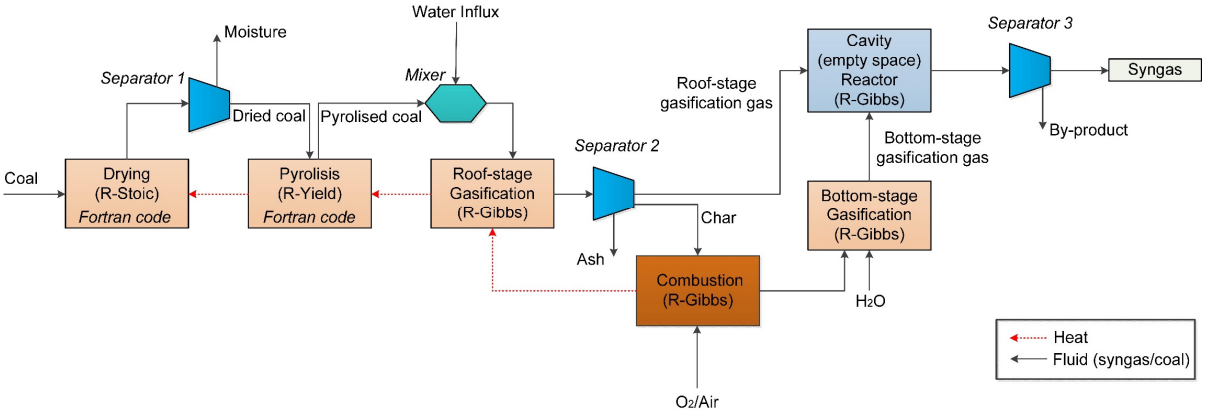


Fig. 4. Chemical process model for the simulation of the CRIP subsurface layout.

However, in contrast to the LVW process model, the more controllable rate of cavity growth results in a better regulated water influx from the surrounding strata, which might mean that additional steam requirements have to be met by steam injection (i.e. $H_2O$) in order to sustain the bottom-stage gasification.

## 4. Results – Sensitivity Analysis

Model simulations were performed with varying operational parameters in order to understand the effect of each parameter on the final product and validate the model performance using experimental data. Relevant experimental work focusing on the UCG process and carried out by Stanczyk et al. [13] was used to calibrate the process models developed. The experiments used Polish hard coal to carry out a two stage gasification process with oxygen and steam reagents supplied alternately in a surface (ex-situ) experimental unit designed to simulate the underground conditions. The surface (ex-situ) reactor is designed such that both the coal seam and the surrounding rock layers are represented and its external dimensions are 3.0 m (length), 1.4 m (width) and 1.5 m (height). The reactor experiment used to calibrate the models presented here [13] lasted approximately 7 days, with average hourly gas yields of 7.8 $m^3$ /h and 9.2 $m^3$ /h for the oxygen and the steam gasification stages, respectively, and a hydrogen concentration of 40–50% [13].

The molar yield composition and the amount of produced syngas were found to be the two most important parameters that allowed the calibration of modeling efforts with the experimental data. Decisive operational parameters were the temperature and pressure conditions as well as the composition and proportions of the gasifying agents. In addition, a qualitative sensitivity analysis was conducted by setting the modeling results that achieve the highest correlation with the experimental outcomes as reference points and implementing incremental changes on the operational parameters.

### *4.1. Comparison of Experimental and Modeling Results*

Table 1 presents the proximate and ultimate analysis of the coal utilised in the validation and sensitivity analysis. For consistency, the modelling studies reported here were performed using as a guide the experimental design reported by Stancyk et al [13] and for the same coal characteristics.

The experimental work conducted by Stanczyk et al. [13] and used in the process model calibration here focused on UCG gasification for hydrogen production. The results of that research work were categorised into three stages

Table 1. Characteristics of coal (after Stanczyk et al. [13]).

| Parameter | Value |
|---|---|
| *Proximate analysis ( % w/w, dry basis)* | |
| Fixed carbon | 64.87 |
| Volatile material | 32.89 |
| Ash | 2.24 |
| *Ultimate analysis (% w/w, dry basis)* | |
| Carbon | 85.09 |
| Hydrogen | 5.01 |
| Nitrogen | 1.17 |
| Sulfur | 0.28 |
| Ash | 2.24 |
| Oxygen | 6.21 |
| *High Heating Value (dry basis, kJ/kg)* | 35,087 |
| *Moisture (% w/w)* | 1.55 |

Table 2. Process modelling results using the LVW and CRIP models developed and comparison with experimental data.

| | Molar yields (%) | | | | Gas production rate ($m^3$/h) |
|---|---|---|---|---|---|
| | $H_2$ | CO | $CO_2$ | $CH_4$ | |
| Modelling results – *LVW Process Model* | 56.2 | 17.8 | 13.1 | 9.9 | 9.12 |
| – *CRIP Process Model* | 55.9 | 18.0 | 13.2 | 9.8 | 8.65 |
| Experimental results – *Stanczyk et al.[13]* | 53.8 | 15.8 | 14.4 | 9.8 | ~ 8.5 (range 5-12) |

(i.e. i) initiation ii) basic gasification iii) termination) depending on the time stage of the experiment. The modelling work of this paper opted to simulate the basic gasification process that had the most stable performance during the whole experiment. The modelling conditions include ambient pressure and temperatures at around 1,100°C, similar to the experimental conditions. In addition, the experimental basic gasification process consisted of two periodic stages of, firstly, oxygen injection and, then, steam supply. As a result, an accurate comparison between the modelling and the experimental results requires the fulfilment of both stages for the whole period. Consequently, the experimental results after the steam injection stage are compared with the modelling outputs, as presented in Table 2.

The high correlation of the experimental and modelling results indicates the reliability of the chemical process models developed, which is important considering that this was achieved using oxygen and steam inputs similar to the experimental values. Specifically, the assumed oxygen and steam supplies used in the process simulations using the models developed (4.96 $m^3$/h and 6.21 $m^3$/h respectively) are comparable and within the range of the corresponding experimental conditions (2-5 $m^3$/h and 6.2 $m^3$/h [13]).

### *4.2. Sensitivity Analyses*

The sensitivity analyses aimed to evaluate how changes in the operational parameters could affect the simulation outcomes. The two criteria used in the evaluation were: i) the energy efficiency ii) and the carbon efficiency. The energy efficiency evaluates how the produced syngas composition is affected by changes in the operational parameters and how this effect is reflected on the heating value of the produced syngas. The energy efficiency is calculated using Equation (1) [30-31]:

$$energy\_eff = \frac{Q_{syngas} \times V_{syngas}}{M_{coal} \times HHV_{coal}} \quad (1)$$

Where $V_{syngas}$ represents the volume ($Nm^3$) of the produced syngas on a dry basis; with regards to the coal used $M_{coal}$ and $HHV_{coal}$ represent the mass (kg) and the high heating value (kJ/kg) respectively. $Q_{syngas}$ (kJ/$Nm^3$) represents the heating value of the generated syngas and was calculated using Equation (2) [31]:

$$Q_{syngas} = \frac{119950.4 \times n_{H_2} + 10103.9 \times n_{CO} + 50009.3 \times n_{CH_4}}{V_{syngas}} \quad (2)$$

Where $n_{H_2}$, $n_{CO}$ and $n_{CH_4}$ represent the molar yields (%) of the corresponding components in the produced syngas on a dry basis.

The second performance indicator used was the carbon efficiency, defined as the fraction of carbon in the final product-syngas as compared to the amount of carbon in the coal gasified, Equation (3), which provides a measure of the success for coal resource conversion [27].

$$carbon\_eff = \frac{M_{carbon\,in\,syngas}}{M_{carbon\,in\,coal}} \quad (3)$$

Where $M_{carbon\ in\ syngas}$ and $M_{carbon\ in\ coal}$ represent the mass (kg) of carbon component in the generated syngas and the utilised coal respectively. It should be noted that this performance indicator refers to the chemical reaction conversion process only and does not consider the requirements of gasifier panel layout at field scale.

The performance indicators results presented below investigate the qualitative effect of a single process parameter change on the energy and carbon efficiencies for each of the UCG gasifier designs considered in this work.

In order to widen the scope of the research conducted here in terms of $CO_2$ storage (or reliance on storage), such that conversion to much valuable chemical feedstock is also treated as a means of mitigating $CO_2$ emissions in situ and transform the product for alternative end uses, an additional sensitivity test using $CO_2$ as an input together with the chemical process reagents, is also considered.

Table 3 outlines the results for the LVW process model developed. It is shown that higher $O_2$ input increases the carbon efficiency, while reducing the energy efficiency. The reason is that, although the higher $O_2$ input increases the combustion temperature, an increasing proportion of the injected $O_2$ is also collected in the final product gas and, as a result, decreases the molar yield of the $H_2$ component. Moreover, in the case of increasing $CO_2$ input, the combustion temperature decreases while the proportion of $CO_2$ in the collected syngas product also increases. As a result the $H_2$, CO and $CH_4$ molar yields decrease, which, in combination with the increased carbon efficiency, indicate that more coal is gasified, while the quality of the produced syngas deteriorates. Overall, Table 3 indicates that although increases of temperature, pressure or of gasification agents' proportions might improve the coal resource utilisation rate (carbon efficiency) this does not necessarily lead to improved syngas quality.

Table 3. Sensitivity analysis – LVW process model (⇧ = increase, ⇩ = decrease).

| *Parameters* | *Energy efficiency* | *Carbon efficiency* |
|---|---|---|
| As gasification temperature increases | ⇧ | ⇧ |
| As pressure increases | ⇩ | ⇧ |
| As $O_2$ input increase | ⇩ | ⇧ |
| As $CO_2$ input increase | ⇩ | ⇧ |
| As water influx increases | ⇩ | ⇧ |

The qualitative sensitivity analysis conducted for the CRIP process model is presented in Table 4 using the two stage gasification process with $O_2$ initially and then steam. It is noted that by increasing either the roof or the bottom stage gasification temperature, the CO and $H_2$ proportions in the final syngas product increase in contrast to the $CH_4$ proportion that decreases. This result is in good agreement with literature on UCG chemistry [5, 33] and chemical processes principles [34]. Overall, both the energy and the carbon efficiencies increase with temperature increase, although implementing a high gasification temperature requires the development of even higher combustion temperature.

The increase of the operational pressure in both the LVW and CRIP process models cause decrease of energy efficiency as the heating value significantly deteriorates due to the decreasing $H_2$ proportions, despite the increasing $CH_4$ content. This $CH_4$ increase as pressure increases is also in good agreement with UCG chemistry gasification studies [5, 33]. However, the carbon efficiency in the CRIP process model increases with pressure increase; in contrast to the LVW process model, where carbon efficiency decreases. This indicates that in the CRIP model the process occurs more rapidly, leaving a lot of coal mass not utilised; whereas with the LVW process model the gasification runs more efficiently, allowing for more coal to be consumed.

Table 4. Sensitivity analysis – CRIP process model (⇧ = increase, ⇩ = decrease).

| *Parameters* | *Energy efficiency* | *Carbon efficiency* |
|---|---|---|
| As roof-stage gasification temperature increases | ⇧ | ⇧ |
| As bottom-stage gasification temperature increases | ⇧ | ⇧ |
| As pressure increases | ⇩ | ⇩ |
| As $O_2$ input increase | ⇩ | ⇧ |
| As $CO_2$ input increase | ⇩ | ⇧ |
| As water influx increases | ⇩ | ⇧ |
| As injected $H_2O$ increases | ⇧ | ⇧ |

Finally, increase in the water influx from the surrounding strata has a negative effect in the energy efficiency for both LVW and CRIP models since it decreases the CO and $H_2$ proportions in the generated syngas (although it also causes a slight increase in the $CH_4$ of the syngas). However, increase in the injected $H_2O$ in the bottom stage gasification causes increase of the energy efficiency due to the higher $H_2$ content of the collected syngas. The reason for the $H_2$ increase is that the bottom stage gasification is conducted at high temperature and under these conditions $H_2$ formation is favoured over $CH_4$. As a result, regulated steam presence in the bottom stage gasification could act beneficially for the heating value of the produced syngas.

## 5. Conclusions

The research reported in this paper coupled chemical process modelling with UCG specific subsurface layouts. It facilitated the simulation of the end-product composition using LVW and CRIP designs allowing the evaluation of the produced syngas quality. In addition, the organisation of the UCG process in different temperature/reactions zones facilitated the comparison between UCG and surface gasification processes by allowing the use of Aspen Plus® software tool. This tool has a proven record of use in the chemicals industry and the research described in this paper used this proven capability for UCG chemical process modelling. The development of different model configurations for specific subsurface layouts (LVW, CRIP) assisted in understanding the operational differences between the UCG geometries and how their distinct operational characteristics are reflected in the resulting UCG syngas chemistry. Although the work presented here does not yet consider important processes like fluid flow or cavity growth, it provides an important building block as part of an integrated UCG model development. The dedicated chemical process modelling, as detailed in this paper, should be included in an integrated UCG model in order to analyse the effect of changes in the operational parameters (e.g. pressure, temperature, type of injected reagents) on the final gas product. In addition, the integration of such chemical process modelling would enhance accuracy in the subsequent UCG models (e.g. hydro-mechanical) by providing reliable and essential information.

## Acknowledgements

This research is receiving funding from the European Union's Seventh Framework Programme for research, technological development and demonstration under grant agreement No. 608517 ("Technology Options for Coupled Underground Coal Gasification and $CO_2$ Capture and Storage, TOPS").

## References

[1] World Energy Council, Coal, in: World Energy Resources: 2013 Survey, 2013, pp. 1.32.
[2] J.C. Fair, O.A. Larson, H.H. Hasiba, An evaluation of in situ coal gasification, Energy, 1 (1976) 77-94.
[3] R. Upadhye, E. Burton, F. J., Science and technology gaps in underground coal gasification, in, University of California, Lawrence Livermore National Laboratory, Livermore, CA, 2006, pp. 15.
[4] P. Younger, Hydrogeological and Geomechanical Aspects of Underground Coal Gasification and its Direct Coupling to Carbon Capture and Storage, Mine Water Environ, 30 (2011) 127-140.

[5] D.W. Gregg, T.F. Edgar, Underground coal gasification, AIChE Journal, 24 (1978) 753-781.
[6] S. Shackley, S. Mander, A. Reiche, Public perceptions of underground coal gasification in the United Kingdom, Energy Policy, 34 (2006) 3423-3433.
[7] S. Daggupati, R.N. Mandapati, S.M. Mahajani, A. Ganesh, A.K. Pal, R.K. Sharma, P. Aghalayam, Compartment Modeling for Flow Characterization of Underground Coal Gasification Cavity, Industrial & Engineering Chemistry Research, 50 (2011) 277-290.
[8] S. Daggupati, R.N. Mandapati, S.M. Mahajani, A. Ganesh, R.K. Sapru, R.K. Sharma, P. Aghalayam, Laboratory studies on cavity growth and product gas composition in the context of underground coal gasification, Energy, 36 (2011) 1776-1784.
[9] DTI, Directional drilling in coal, in: Technology Status Report, dti, Cleaner Fossil Fuels Programme, 2005, pp. 28.
[10] A. Khadse, M. Qayyumi, S. Mahajani, P. Aghalayam, Underground coal gasification: A new clean coal utilization technique for India, Energy, 32 (2007) 2061-2071.
[11] M. Wiatowski, K. Stańczyk, J. Świądrowski, K. Kapusta, K. Cybulski, E. Krause, J. Grabowski, J. Rogut, N. Howaniec, A. Smoliński, Semi-technical underground coal gasification (UCG) using the shaft method in Experimental Mine "Barbara", Fuel, 99 (2012) 170-179.
[12] E. Burton, F. J., R. Upadhye, Best Practices in Underground Coal Gasification, in, University of California, Lawrence Livermore National Laboratory, Livermore, CA, 2007, pp. 119.
[13] K. Stańczyk, K. Kapusta, M. Wiatowski, J. Świądrowski, A. Smoliński, J. Rogut, A. Kotyrba, Experimental simulation of hard coal underground gasification for hydrogen production, Fuel, 91 (2012) 40-50.
[14] P. Aghalayam, Underground coal gasification: a clean coal technology, in: Handbook of combustion, Wiley-VCH, New York, 2010, pp. 257–275.
[15] A. Sharaf, J. Mmbaga, Gupta, R.E. Hayes, Modelling Cavity Growth during Underground Coal Gasification, in: Comsol Conference, Boston 2011.
[16] G. Perkins, V. Sahajwalla, A Mathematical Model for the Chemical Reaction of a Semi-infinite Block of Coal in Underground Coal Gasification, Energy & Fuels, 19 (2005) 1679-1692.
[17] G. Perkins, V. Sahajwalla, Steady-State Model for Estimating Gas Production from Underground Coal Gasification, Energy & Fuels, 22 (2008) 3902-3914.
[18] J. Liang, S.-q. Liu, L. Yu, Trial study on underground coal gasification of abandoned coal resource, in: Proceedings of the '99 International Symposium on Mining Science and Technology, A A Balkema, 1999, pp. 271-275.
[19] D.J. Roddy, P.L. Younger, Underground coal gasification with CCS: a pathway to decarbonising industry, Energy & Environmental Science, 3 (2010) 400-407.
[20] G.X. Wang, Z.T. Wang, B. Feng, V. Rudolph, J.L. Jiao, Semi-industrial tests on enhanced underground coal gasification at Zhong-Liang-Shan coal mine, Asia-Pacific Journal of Chemical Engineering, 4 (2009) 771-779.
[21] H. Nourozieh, M. Kariznovi, Z. Chen, J. Abedi, Simulation study of underground coal gasification in Alberta reservoirs: geological structure and process modeling, Energy & Fuels, 24 (2010) 3540-3550.
[22] E. Shafirovich, A. Varma, Underground Coal Gasification: A Brief Review of Current Status, Industrial & Engineering Chemistry Research, 48 (2009) 7865-7875.
[23] S. Self, B. Reddy, M. Rosen, Review of underground coal gasification technologies and carbon capture, Int J Energy Environ Eng, 3 (2012) 1-8.
[24] L.H. Yang, X.L. Pang, S.Q. Liu, F. Chen, Temperature and Gas Pressure Features in the Temperature-control Blasting Underground Coal Gasification, Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, 32 (2010) 1737-1746.
[25] Aspen Plus, Getting started modelling processes with solids, in, 2009.
[26] S. Begum, M. Rasul, D. Akbar, N. Ramzan, Performance Analysis of an Integrated Fixed Bed Gasifier Model for Different Biomass Feedstocks, Energies, 6 (2013) 6508-6524.
[27] C. Chen, Y.-q. Jin, J.-h. Yan, Y. Chi, Simulation of municipal solid waste gasification for syngas production in fixed bed reactors, J. Zhejiang Univ. Sci. A, 11 (2010) 619-628.
[28] J. Preciado, J. Ortiz-Martinez, J. Gonzalez-Rivera, R. Sierra-Ramirez, G. Gordillo, Simulation of Synthesis Gas Production from Steam Oxygen Gasification of Colombian Coal Using Aspen Plus®, Energies, 5 (2012) 4924-4940.
[29] F. Emun, M. Gadalla, T. Majozi, D. Boer, Integrated gasification combined cycle (IGCC) process simulation and optimization, Computers & Chemical Engineering, 34 (2010) 331-338.
[30] N. Ramzan, A. Ashraf, S. Naveed, A. Malik, Simulation of hybrid biomass gasification using Aspen plus: A comparative performance analysis for food, municipal solid and poultry waste, Biomass and Bioenergy, 35 (2011) 3962-3969.
[31] Y. Wang, W. Dong, L. Dong, J. Yue, S. Gao, T. Suda, G. Xu, Production of middle caloric fuel gas from coal by dual-bed gasification technology, Energy & Fuels, 24 (2010) 2985-2990.
[32] Y.S. Teh, G.P. Rangaiah, A Study of Equation-Solving and Gibbs Free Energy Minimization Methods for Phase Equilibrium Calculations, Chemical Engineering Research and Design, 80 (2002) 745-759.
[33] C. Von Fredersdorff, M. Elliott, Coal Gasification, in: H.H. Lowry (Ed.) Chemistry of coal utilization. Second supplementary volume, Wiley, New York, 1963, pp. Medium: X; Size: Pages: 2395.
[34] R. Felder, R. Rousseau, Elementary Principles of Chemical Processes (3rd edition), John Wiley & Sons, New York, 2004.